



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:28 AM GMT

PDB ID : 3II9
Title : Crystal structure of glutaryl-coa dehydrogenase from Burkholderia pseudomallei at 1.73 Angstrom
Authors : Ismagilov, R.F.; Li, L.; Du, W.B.; Staker, B.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D); Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-07-31
Resolution : 1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

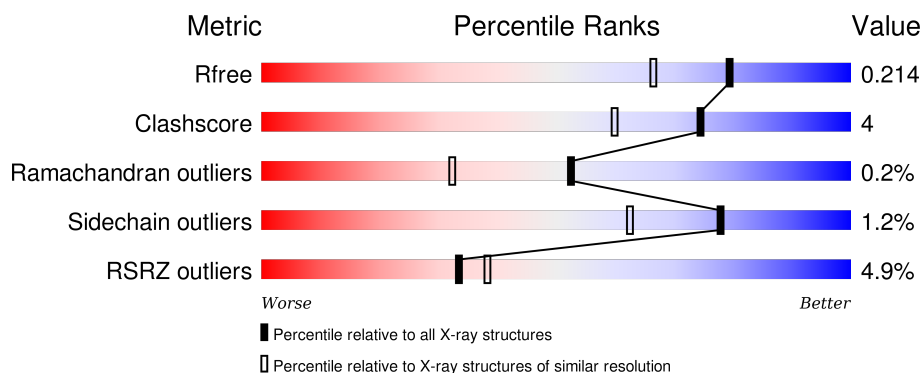
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div>5%</div> <div>91%</div> <div>6% ..</div> </div>
1	B	396	<div> <div>5%</div> <div>90%</div> <div>5% ..</div> </div>
1	C	396	<div> <div>4%</div> <div>89%</div> <div>9% .</div> </div>
1	D	396	<div> <div>4%</div> <div>90%</div> <div>8% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	C	397	-	-	-	X
2	PEG	D	398	-	-	-	X
4	PGE	A	398	-	-	-	X
4	PGE	C	396	-	-	-	X
5	PG4	C	401	-	-	-	X
6	GOL	B	398	-	-	-	X
6	GOL	C	402	-	-	-	X
6	GOL	D	396	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12893 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	3	0
			2987	1890	524	556	17			
1	B	379	Total	C	N	O	S	0	2	0
			2909	1843	516	533	17			
1	C	388	Total	C	N	O	S	0	5	0
			3006	1907	533	549	17			
1	D	386	Total	C	N	O	S	0	1	0
			2963	1876	526	544	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q3JP94
B	0	SER	-	expression tag	UNP Q3JP94
C	0	SER	-	expression tag	UNP Q3JP94
D	0	SER	-	expression tag	UNP Q3JP94

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

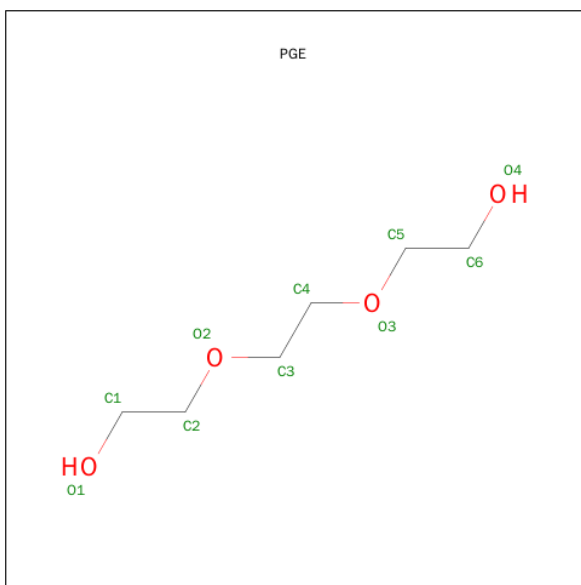


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	230	Total	O	0	0
			230	230		
7	B	218	Total	O	0	0
			218	218		
7	C	239	Total	O	0	0
			239	239		

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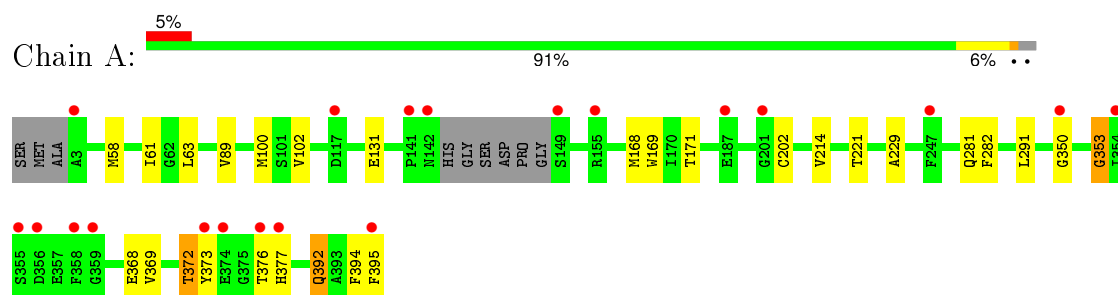
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	220	Total 220	O 220	0	0

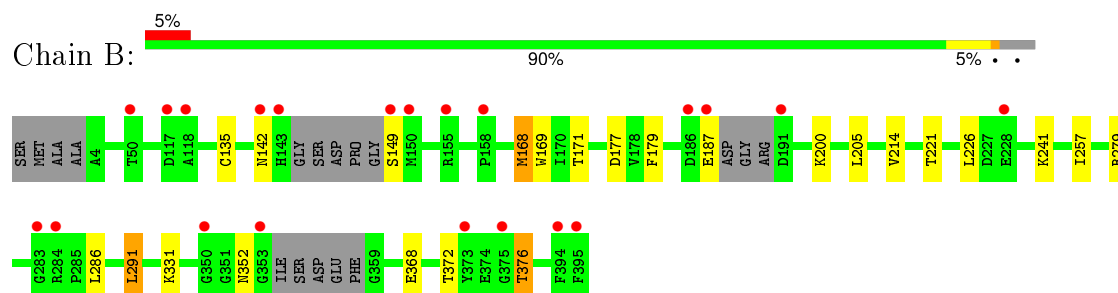
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

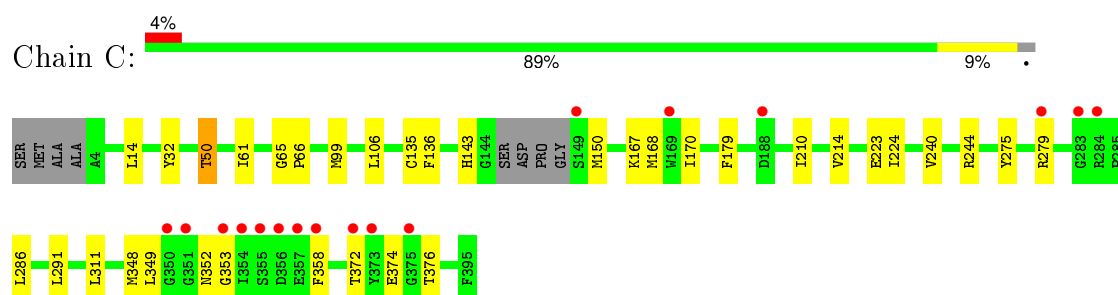
- Molecule 1: Glutaryl-CoA dehydrogenase



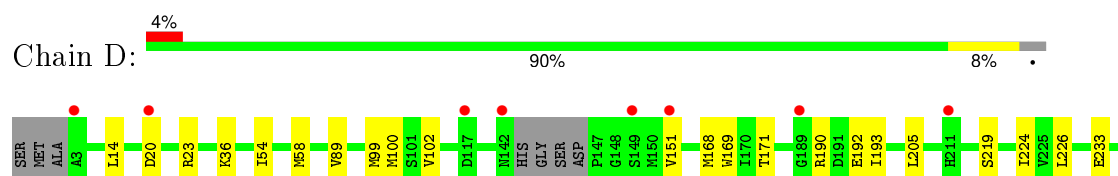
- Molecule 1: Glutaryl-CoA dehydrogenase

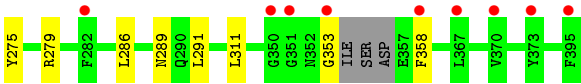


- Molecule 1: Glutaryl-CoA dehydrogenase



- Molecule 1: Glutaryl-CoA dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.97Å 141.27Å 84.01Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	40.23 – 1.74 39.87 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.23-1.74) 98.8 (39.87-1.74)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.170 , 0.196 0.188 , 0.214	Depositor DCC
R_{free} test set	8866 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.9	EDS
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 177387 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12893	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, GOL, MG, PGE, PG4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/3048	0.60	0/4121
1	B	0.43	0/2964	0.59	0/4005
1	C	0.43	0/3070	0.60	0/4150
1	D	0.44	0/3021	0.60	0/4080
All	All	0.44	0/12103	0.60	0/16356

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	358	PHE	Peptide
1	D	358	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2987	0	2971	31	0
1	B	2909	0	2899	18	0
1	C	3006	0	2989	39	0
1	D	2963	0	2956	24	0
2	A	7	0	10	1	0
2	C	7	0	10	0	0
2	D	14	0	20	0	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	14	0	0
4	C	10	0	14	0	0
5	B	26	0	36	0	0
5	C	13	0	18	0	0
6	B	6	0	8	0	0
6	C	12	0	16	1	0
6	D	12	0	16	1	0
7	A	230	0	0	2	0
7	B	218	0	0	3	0
7	C	239	0	0	2	0
7	D	220	0	0	1	0
All	All	12893	0	11977	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135[B]:CYS:SG	1:C:170[B]:ILE:HG22	1.70	1.31
1:C:135[B]:CYS:SG	1:C:170[B]:ILE:CG2	2.37	1.11
1:A:376:THR:HG21	1:C:286:LEU:HD23	1.59	0.82
1:A:131:GLU:OE1	7:A:611:HOH:O	1.99	0.79
1:C:374:GLU:OE1	7:C:522:HOH:O	2.07	0.72
1:B:291:LEU:HD12	1:C:291:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:HA	1:B:221[B]:THR:HG22	1.74	0.69
1:C:170[B]:ILE:HD13	1:C:224:ILE:HD12	1.79	0.64
1:A:89:VAL:HG21	1:A:100:MET:HE1	1.78	0.64
1:C:167:LYS:HB2	1:C:170[B]:ILE:HD11	1.80	0.63
1:D:99:MET:HE2	1:D:219:SER:HA	1.79	0.62
1:C:135[A]:CYS:SG	1:C:179:PHE:CD1	2.93	0.61
1:B:214:VAL:HG23	1:D:353:GLY:HA3	1.82	0.61
1:A:350:GLY:HA2	1:C:372:THR:OG1	2.01	0.60
1:A:291:LEU:HD23	1:D:291:LEU:HD23	1.83	0.60
1:D:20:ASP:OD2	1:D:23:ARG:NH1	2.35	0.59
1:D:54:ILE:HG22	1:D:58:MET:CE	2.33	0.59
1:A:58:MET:HE1	1:A:100:MET:HE2	1.84	0.58
1:D:205:LEU:HD13	1:D:226:LEU:HD21	1.84	0.58
1:C:170[B]:ILE:HD13	1:C:224:ILE:CD1	2.34	0.57
1:B:205:LEU:HD13	1:B:226:LEU:HD21	1.86	0.56
1:D:36:LYS:HZ2	6:D:396:GOL:H32	1.71	0.56
1:C:143:HIS:NE2	1:C:150:MET:HB3	2.21	0.56
1:B:376:THR:HG21	1:D:286:LEU:CD1	2.36	0.56
1:B:168:MET:HG3	1:B:169:TRP:CD1	2.40	0.56
1:A:353:GLY:HA3	1:C:214:VAL:HG23	1.87	0.55
1:B:257:ILE:HG21	1:B:331:LYS:HE2	1.88	0.54
1:C:170[B]:ILE:HD13	1:C:224:ILE:CG1	2.38	0.54
1:A:376:THR:O	1:A:376:THR:HG22	2.08	0.54
1:A:168:MET:HG3	1:A:169:TRP:CD1	2.43	0.54
1:D:99:MET:CE	1:D:219:SER:HA	2.38	0.54
1:D:205:LEU:HD13	1:D:226:LEU:CD2	2.37	0.54
1:C:374:GLU:HB2	1:C:376:THR:CG2	2.38	0.53
1:A:89:VAL:HG21	1:A:100:MET:CE	2.39	0.53
1:C:14:LEU:CD1	1:C:311:LEU:HD22	2.39	0.52
1:A:376:THR:HG23	1:C:348[B]:MET:O	2.09	0.52
1:C:374:GLU:HB2	1:C:376:THR:HG23	1.91	0.52
1:A:372:THR:OG1	1:C:349:LEU:O	2.27	0.52
1:D:89:VAL:HG21	1:D:100[A]:MET:SD	2.50	0.52
1:A:58:MET:CE	1:A:100:MET:CE	2.88	0.52
1:C:210:ILE:HD11	1:C:223:GLU:HG3	1.92	0.51
1:C:135[B]:CYS:SG	1:C:170[B]:ILE:HG21	2.47	0.50
1:C:14:LEU:HD11	1:C:311:LEU:HD22	1.93	0.50
1:A:214[A]:VAL:HG23	1:C:353:GLY:HA3	1.93	0.50
1:A:350:GLY:HA2	1:C:372:THR:CB	2.41	0.50
1:D:54:ILE:HG22	1:D:58:MET:HE1	1.94	0.49
1:B:205:LEU:HD13	1:B:226:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:TYR:CZ	1:D:279:ARG:HG3	2.48	0.49
1:C:167:LYS:CB	1:C:170[B]:ILE:HD11	2.43	0.49
1:B:214:VAL:HG23	1:D:353:GLY:CA	2.43	0.48
1:B:291:LEU:CD1	1:C:291:LEU:HD23	2.42	0.47
1:C:170[B]:ILE:HD13	1:C:224:ILE:HG13	1.95	0.47
1:C:50:THR:HG21	1:C:99:MET:SD	2.54	0.47
1:A:281:GLN:HG2	1:A:282:PHE:CD2	2.49	0.47
1:A:376:THR:CG2	1:A:376:THR:O	2.62	0.46
1:B:200:LYS:NZ	7:B:1152:HOH:O	2.48	0.46
1:A:58:MET:HE1	1:A:100:MET:CE	2.44	0.46
1:A:102:VAL:HG21	1:A:171:THR:HB	1.97	0.46
1:B:376:THR:HG21	1:D:286:LEU:HD13	1.96	0.46
1:D:193:ILE:HD12	1:D:193:ILE:H	1.80	0.46
1:B:376:THR:HG21	1:D:286:LEU:HD11	1.97	0.46
1:D:102:VAL:HG21	1:D:171:THR:HB	1.98	0.45
1:C:106:LEU:HD11	6:C:399:GOL:H31	1.98	0.45
1:D:54:ILE:HG22	1:D:58:MET:HE2	1.99	0.45
1:A:58:MET:CE	1:A:100:MET:HE2	2.46	0.45
1:A:392:GLN:OE1	1:A:394:PHE:N	2.49	0.45
1:C:244:ARG:NH1	7:C:451:HOH:O	2.51	0.44
1:C:210:ILE:HD11	1:C:223:GLU:CG	2.47	0.43
1:A:369:VAL:O	1:A:372:THR:HG22	2.19	0.43
1:A:58:MET:HE3	1:A:100:MET:HE3	2.01	0.43
1:B:368:GLU:OE1	7:B:780:HOH:O	2.19	0.43
1:C:168[A]:MET:O	1:C:170[A]:ILE:HG12	2.19	0.43
1:A:376:THR:HG23	1:C:348[A]:MET:O	2.17	0.43
1:C:32:TYR:HB2	1:C:61:ILE:HD13	2.01	0.43
1:B:135:CYS:SG	1:B:179:PHE:CD1	3.12	0.43
1:C:65:GLY:N	1:C:66:PRO:HD3	2.33	0.43
1:A:58:MET:HE3	1:A:100:MET:CE	2.48	0.43
1:D:14:LEU:CD1	1:D:311:LEU:HD22	2.49	0.43
1:A:368:GLU:OE1	7:A:905:HOH:O	2.21	0.42
1:A:61:ILE:HD11	1:A:63:LEU:HD11	2.01	0.42
1:A:171:THR:HA	1:A:221[B]:THR:HG22	2.01	0.42
1:C:275:TYR:CZ	1:C:279:ARG:HG3	2.54	0.42
1:A:214[B]:VAL:HG12	2:A:396:PEG:H21	2.01	0.42
1:C:168[A]:MET:O	1:C:170[A]:ILE:CD1	2.68	0.42
1:B:372:THR:HG23	7:D:422:HOH:O	2.20	0.41
1:C:136:PHE:O	1:C:170[A]:ILE:HD12	2.20	0.41
1:B:279:ARG:O	1:B:286:LEU:HD13	2.20	0.41
1:B:177:ASP:OD2	7:B:652:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:MET:HG3	1:D:169:TRP:CD1	2.55	0.41
1:D:205:LEU:HD11	1:D:224:ILE:HG23	2.03	0.41
1:D:151:VAL:HG12	1:D:151:VAL:O	2.21	0.41
1:A:202:CYS:SG	1:A:229:ALA:HB1	2.61	0.41
1:C:240:VAL:HG23	1:C:244:ARG:NH1	2.36	0.40
1:A:377:HIS:NE2	1:C:291:LEU:HD12	2.37	0.40
1:D:289:ASN:OD1	1:D:291:LEU:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/396 (98%)	378 (98%)	7 (2%)	1 (0%)	46	26
1	B	373/396 (94%)	367 (98%)	5 (1%)	1 (0%)	46	26
1	C	389/396 (98%)	380 (98%)	8 (2%)	1 (0%)	46	26
1	D	381/396 (96%)	374 (98%)	7 (2%)	0	100	100
All	All	1529/1584 (96%)	1499 (98%)	27 (2%)	3 (0%)	52	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ASN
1	C	352	ASN
1	A	353	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/313 (98%)	304 (99%)	4 (1%)	76	60
1	B	297/313 (95%)	290 (98%)	7 (2%)	57	31
1	C	306/313 (98%)	305 (100%)	1 (0%)	94	91
1	D	303/313 (97%)	300 (99%)	3 (1%)	82	69
All	All	1214/1252 (97%)	1199 (99%)	15 (1%)	78	62

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	THR
1	A	373	TYR
1	A	392	GLN
1	A	395	PHE
1	B	142	ASN
1	B	149	SER
1	B	168	MET
1	B	187	GLU
1	B	241	LYS
1	B	291	LEU
1	B	376	THR
1	C	50	THR
1	D	190	ARG
1	D	192	GLU
1	D	233	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	47	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	A	396	-	6,6,6	0.43	0	5,5,5	0.22	0
4	PGE	A	398	-	9,9,9	0.45	0	8,8,8	0.27	0
5	PG4	B	396	-	12,12,12	0.46	0	11,11,11	0.21	0
5	PG4	B	397	-	12,12,12	0.46	0	11,11,11	0.36	0
6	GOL	B	398	-	5,5,5	0.35	0	5,5,5	0.22	0
4	PGE	C	396	-	9,9,9	0.47	0	8,8,8	0.26	0
2	PEG	C	397	-	6,6,6	0.47	0	5,5,5	0.26	0
6	GOL	C	399	-	5,5,5	0.37	0	5,5,5	0.14	0
5	PG4	C	401	-	12,12,12	0.56	0	11,11,11	0.57	0
6	GOL	C	402	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	D	396	-	5,5,5	0.37	0	5,5,5	0.28	0
6	GOL	D	397	-	5,5,5	0.36	0	5,5,5	0.31	0
2	PEG	D	398	-	6,6,6	0.41	0	5,5,5	0.26	0
2	PEG	D	399	-	6,6,6	0.48	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	396	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	398	-	-	0/7/7/7	0/0/0/0
5	PG4	B	396	-	-	0/10/10/10	0/0/0/0
5	PG4	B	397	-	-	0/10/10/10	0/0/0/0
6	GOL	B	398	-	-	0/4/4/4	0/0/0/0
4	PGE	C	396	-	-	0/7/7/7	0/0/0/0
2	PEG	C	397	-	-	0/4/4/4	0/0/0/0
6	GOL	C	399	-	-	0/4/4/4	0/0/0/0
5	PG4	C	401	-	-	0/10/10/10	0/0/0/0
6	GOL	C	402	-	-	0/4/4/4	0/0/0/0
6	GOL	D	396	-	-	0/4/4/4	0/0/0/0
6	GOL	D	397	-	-	0/4/4/4	0/0/0/0
2	PEG	D	398	-	-	0/4/4/4	0/0/0/0
2	PEG	D	399	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	396	PEG	1	0
6	C	399	GOL	1	0
6	D	396	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/396 (97%)	0.31	20 (5%) 31 36	2, 15, 23, 35	0
1	B	379/396 (95%)	0.28	21 (5%) 29 33	7, 16, 26, 37	0
1	C	388/396 (97%)	0.24	17 (4%) 38 44	8, 16, 27, 33	0
1	D	386/396 (97%)	0.26	17 (4%) 38 44	8, 16, 27, 37	0
All	All	1540/1584 (97%)	0.27	75 (4%) 33 38	2, 16, 26, 37	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	ILE	10.1
1	C	375	GLY	9.9
1	A	395	PHE	7.4
1	D	350	GLY	6.8
1	C	351	GLY	6.8
1	D	395	PHE	6.0
1	D	3	ALA	6.0
1	A	3	ALA	5.9
1	B	395	PHE	5.7
1	A	149	SER	5.5
1	B	142	ASN	5.3
1	A	358	PHE	5.2
1	A	377	HIS	4.7
1	C	358	PHE	4.7
1	A	354	ILE	4.6
1	B	149	SER	4.6
1	D	142	ASN	4.2
1	A	142	ASN	4.1
1	A	355	SER	4.0
1	C	356	ASP	3.9
1	C	373	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLY	3.9
1	B	187	GLU	3.9
1	C	169[A]	TRP	3.8
1	D	373	TYR	3.8
1	B	143	HIS	3.7
1	B	191	ASP	3.7
1	A	141	PRO	3.7
1	D	358	PHE	3.6
1	B	158	PRO	3.5
1	B	186	ASP	3.3
1	A	350	GLY	3.2
1	C	355	SER	3.2
1	B	353	GLY	3.2
1	D	351	GLY	3.1
1	A	187	GLU	3.0
1	A	356	ASP	3.0
1	A	373	TYR	2.8
1	C	283	GLY	2.8
1	D	282	PHE	2.8
1	A	359	GLY	2.8
1	A	155	ARG	2.8
1	C	350	GLY	2.7
1	B	50	THR	2.7
1	D	189	GLY	2.6
1	C	188	ASP	2.5
1	B	284	ARG	2.5
1	B	375	GLY	2.5
1	D	149	SER	2.5
1	B	155	ARG	2.5
1	A	117	ASP	2.4
1	B	373	TYR	2.4
1	B	350	GLY	2.4
1	B	283	GLY	2.4
1	B	150	MET	2.3
1	C	357	GLU	2.3
1	A	374	GLU	2.2
1	D	370	VAL	2.2
1	D	211	HIS	2.2
1	C	284	ARG	2.2
1	B	118	ALA	2.2
1	C	149	SER	2.2
1	B	394	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	117	ASP	2.2
1	D	151	VAL	2.2
1	D	20	ASP	2.1
1	B	117	ASP	2.1
1	A	376	THR	2.1
1	D	367	LEU	2.1
1	C	279	ARG	2.1
1	A	247	PHE	2.0
1	C	372	THR	2.0
1	C	353	GLY	2.0
1	D	353	GLY	2.0
1	B	228	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	PG4	C	401	13/13	0.58	0.19	11.08	64,65,66,66	0
4	PGE	A	398	10/10	0.85	0.18	5.27	58,58,59,60	0
6	GOL	C	402	6/6	0.68	0.17	4.41	65,66,67,67	0
2	PEG	D	398	7/7	0.88	0.11	3.82	50,50,52,52	0
6	GOL	B	398	6/6	0.71	0.17	3.36	69,70,71,71	0
6	GOL	D	396	6/6	0.82	0.19	3.08	63,64,64,64	0
4	PGE	C	396	10/10	0.80	0.15	2.26	64,65,65,65	0
2	PEG	C	397	7/7	0.73	0.27	2.04	60,60,61,61	0
5	PG4	B	397	13/13	0.84	0.14	1.20	43,47,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	C	399	6/6	0.80	0.21	1.18	48,49,49,52	0
2	PEG	A	396	7/7	0.90	0.13	0.47	56,57,58,58	0
5	PG4	B	396	13/13	0.87	0.10	0.16	39,40,43,44	0
3	MG	C	398	1/1	0.89	0.14	0.03	38,38,38,38	0
3	MG	A	397	1/1	0.97	0.03	-1.94	28,28,28,28	0
3	MG	D	400	1/1	0.69	0.07	-	61,61,61,61	0
6	GOL	D	397	6/6	0.75	0.21	-	75,75,75,75	0
3	MG	C	400	1/1	0.88	0.09	-	60,60,60,60	0
2	PEG	D	399	7/7	0.69	0.20	-	63,64,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.